CTCMS Workshop on Hybrid Methods in Multiscale Modeling of Materials

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Mads Sorensen (LANL)
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Abstracts

Jayanth Banavar (Penn State)*
Continuum deductions from molecular hydrodynamics

I will present the the results of molecular dynamics simulations o fluids in situations in which the continuum equations of fluid mechanics must be supplemented by information about processes occurring at microscopic scales. Examples include the formulation of boundary conditions, the resolution of singular solutions of the governing equations, and the determination of constitutive relations.

*with Marek Cieplak and Joel Koplik

Alejandro L. Garcia (LBNL and SJSU)*
Adaptive Mesh and Algorithm Refinement using Direct Simulation Monte Carlo

When a large range of scales must be spanned, computational fluid dynamics calculations often employ local mesh refinement so that a fine grid is used only in those regions that require high resolution. However, hydrodynamic formulations break down as the grid spacing approaches the

molecular scale, for example, the mean free path in a gas. This talk will describe Adaptive Mesh and Algorithm Refinement (AMAR), in which a continuum algorithm is replaced by a particle algorithm at the finest grid scale. The coupling between the particle region and the overlaying continuum grid is algorithmically equivalent to that between the fine and coarse levels in mesh refinement. Direct simulation Monte Carlo (DSMC) is used as the particle algorithm embedded within a Godunov-type compressible Navier Stokes solver. Several examples will be presented and compared with purely continuum calculations.

*with John B. Bell, William Y. Crutchfield, and Berni J. Alder

Nicolas G Hadjiconstantinou (LLNL
Hybrid atomistic-continuum formulations for molecular dynamics

We present a hybrid atomistic-continuum computational framework for the treatment of dense fluid problems with emphasis on the coupling of molecular dynamics with continuum (finite element/spectral) methods for problems involving multi-fluid dynamics in the presence of multi-fluid interfaces. The well known moving contact-line problem is used as a validation example. A hybrid solution that employs molecular dynamics close to the walls where molecular effects are important and continuum fluid mechanics in the remainder of the domain (far field region) is obtained. A fully molecular solution of the same problem serves as an exact solution. Various issues related to dense fluid atomistic-continuum techniques are discussed and contrasted to the already existing but less general dilute gas techniques. Numerical considerations are discussed with particular emphasis on efficiency, and a formulation is proposed that reduces computational cost.

David Jacqmin (NASA)
Calculation of Two-Phase Navier-Stokes Flows Using Phase-Field Modeling

This talk will have two parts. I will first discuss some convergence results for phase-field modeling of the fluid dynamics of two-phase incompressible Navier-Stokes flow. The physics and pseudo-physics of phase-field flows will be discussed and how phase-field fluid mechanics converges to classical sharp-interface fluid mechanics. The overall convergence of phase-field numerical modeling is given by a double limit which is a combination of the asymptotics of the approach of the phase-field model to the physics of the exact sharp interface and of the convergence of the numerical methods to the exact solution of the phase-field model. Some definite convergence results have been obtained using a fourth-order compact differencing scheme. The asymptotic rate of convergence for this scheme is approximately first order but the practical convergence rate for affordable grid sizes is considerably faster. The overall convergence rate is set mainly by the rate of convergence of exact phase-field results to exact sharp-interface results. This convergence rate is generally asymptotically proportional to diffuse interface thickness. The second part of the talk will discuss applications, especially moving contact line flows, including dewetting flows, ternary flows with surfactant, and two-phase flows subject to electrical fields.

Li Ju (MIT
Nearly Exact Solution for Coupled Continuum/MD Fluid Simulation

A general statistical approach is described to couple continuum witt MD in fluid simulation. Arbitrary thermodynamic field boundary conditions can be imposed on an MD system while minimally disturbing its particle dynamics. And by acting faraway from the region of interest through a feedback control mechanism, across a buffer zone where the disturbed dynamics are allowed to relax, we can eliminate that disturbance entirely. The field estimator, based on maximum likelihood inference, serves as the detector of the control loop, which infers smooth instantaneous fields from the particle data. The optimal particle controller, defined by an implicit relation, can be proved mathematically to give the correct distribution with least disturbance to the dynamics. A control algorithm compares the estimated current fields with the desired fields at

the boundary and corrects the actions of the faraway controller until they eventually agree. Using this method and a continuum code under the Schwartz iterative domain-decomposition formalism, it provides mutually consistent solution for most steady-state problems where particles in the MD region should have no way to tell any difference with reality. Some illustrative results will be discussed.

Steve Karmesin (LANL)
Computational Frameworks for Multiscale Modeling

There are many problems to be solved when trying to perform reliable computations involving different kinds of physics across one simulation in addition to the purely numerics and physics questions of the validity of the models. I will discuss the POOMA project, a framework of C++ classes for scientific computation, as well as related projects under way in the Advanced Computing Laboratory at LANL and their role in performing very large scale multimaterial calculations for the ASCI program. These tools are being used to provide abstractions to encapsulate some of the repetitive and error-prone tasks associated with large scale parallel computations, including data parallel array and particle sets, and boundary conditions. I will also discuss our current work in progress with encapsulating multithreading, dataflow evaluation and cache optimizations.

George Karniadakis (Brown)
DSMC/Spectral Element modeling for micro-channel gas flows

I will present hybrid algorithms we have developed over the last 10 years for rarefied gas flows in complex micro-geometries. A new high-order boundary condition for the velocity slip and the temperature jump is developed and tested in the Knudsen regime from 0 to 200. The coupling of continuum and particle domains is achieved using the new boundary condition in the buffer region in conjunction with a relaxation type alternating algorithm.

Tim Kaxiras (Harvard)
Multiscale modeling of brittle materials

Application of large stresses to brittle solids can lead to cleavage and crack propagation, or structural transformations and plastic deformation on a macroscopic scale. While these phenomena are ultimately due to changes in the structure at the atomic level, they must be described at macroscopic lengths in order to make contact with experiment, and to account fully for the observed behavior. In covalent solids, this coupling of length scales is made more challenging by the directed and localized nature of the interatomic bonds. We have investigated issues related to multiscale modeling of silicon, a representative brittle solid, in various physical processes like crack propagation under external loading [1] and deformation under an indenter [2]. Results and prospects for future extensions will be discussed.

[1] In collaboration with J. Broughton, F. Abraham, N. Bernstein; see Comp. in Physics 12, 538 (1998).
[2] In collaboration with G. Smith and E. Tadmor; see Phys. Rev. B 59, 235 (1999).

Turab Lookman (LANL and Western Ontario
Multiscale Textures in Elastic Materials

Solid-solid structural phase transitions, especially those with unit cells related by continuous deformations, exhibit a rich variety of temperature/stress induced microtextures. Examples of technologically important materials include shape memory alloys and martensite (e.g. NiTi, FePd, AuCd), ferroelectrics (e.g. BaTiO3), magnetoelastic (e.g. Terfenol-D), etc. I will describe our attempts to provide a unified understanding of twinning, tweed, nucleation pathways and stress loading for the martensitic transition, from a mesoscopic description entirely in strain variables (i.e. primary order parameter). The results based on this Ginsburg-Landau (GL) model

provide the phase transition response of a metallic sub-grain. The parameters of the GL model are determined from microscopic calculations such as MD based on the embedded atom potential method (EAM). This represents a micro to mesoscale length scale bridging. The GL model can subsequently be employed to obtain the constitutive model (i.e. stress-strain relationship) for a sub-grain within a homogenization framework. This embedding of the GL model into a homogenization model represents a meso to macroscopic length scale bridging. The resulting analysis can provide the necessary macroscopic constitutive model that can be used in a finite element code or some other macroscopic (such as micromechanics) structural analysis framework. This work is supported by the US DOE.

Elaine Oran (NRL)
Some Issues for Computing Low-Velocity High-Knudsen Number Flows -- Possibilities from Scaling and Filtering

Microsystem gas flows are usually at a very low velocity (on the order of centimeters/second) and relatively high Knudsen numbers. This is a regime in which both experiments and computations are very difficult. Until recently, no experimental data could be trusted to give the correct values of physical variables. Direct Simulation Monte Carlo (DSMC) computations become either ridiculously expensive simply impossible. To try to "beat the system," or at least get a handle on solutions to these flows, we have been investigating the possibilities of scaling, filtering, and combining DSMC with Navier-Stokes solutions. Progress to date will be reported.

Rob Phillips (Brown)
Atomistic Simulation without All of the Atoms: Constraint and Energetics

A key thread in the quest to construct tractable models of many-particle systems is the quest to eliminate computational overhead in both the spatial and temporal domains. This ambition is more than a computational convenience and reflects the physical idea that in many circumstances only certain important subsets of the full set of spatial degrees of freedom are really doing anything interesting. This talk will describe the linkage of geometric constraints emanating from the finite element method with energetic arguments deriving from atomistic simulation in order to produce models in which degree of freedom elimination can be carried out in a systematic way. Applications to the complex and fully three-dimensional interactions of dislocations will be described with special reference to the role of dislocation junctions in mediating the hardening of crystals as they are subjected to increasing deformation.

Claudio Rebbi (Boston University)
Multiscale problems in particle physics

Particle interactions span multiple scale of energies, ranging from a few tens of MeV to several TeV and beyond. In this talk I will illustrate the emergence of multiple scales in particle interactions, the methods used by particle theorists to cope with these multiple scales and open problems still faced in this field.

Robert E. Rudd (Oxford)*
Coupling of length scales in the dynamics of microsystems

This work studies multi-scale phenomena in silicon and quartz micro-resonators comprising the mechanical components of next-generation Micro-Electro-Mechanical Systems (MEMS). The behavior of next-generation, sub-micron MEMS is determined in part by the interplay between physics at the Angstrom, nanometer and micron scales. As device sizes are reduced below the micron scale, atomistic processes cause systematic deviations from the behavior predicted by continuum elastic theory and finite elements.[1,2] The simulation of these atomistic effects is a challenging problem due to the large number of atoms involved. Our simulations include up to two million atoms in the device itself, and hundreds of millions more are in the proximal regions

of the substrate. A direct, atomistic simulation (MD) of this many atoms is prohibitive, and it would be inefficient. The micron-scale processes in the substrate are well-described by finite elements (FE), and an atomistic description is not required. On the other hand, atomistic processes in the device are inherently coupled to the micron-scale strain fields which extend out into the substrate. In order to capture physical effects at both length scales simultaneously, we have developed a multiple-scale methodology [3,4]. This has been the focus of our DoD HPC Grand Challenge Project on multi-scale simulation.[5] The crucial point to any inhomogeneous multi-scale methodology is the way in which the length-scale domains are coupled. We have employed two approaches: a mean-force boundary condition [3] and a sophisticated coarse-grained coupling [4]. Both approaches give a natural domain decomposition to divide the computational load among parallel processors. The first approach directly couples MD to conventional FE. This is suitable when the FE region is in the far field. The second approach, coarse-grained molecular dynamics (CGMD), is similar to FE, but with scale-dependent constitutive relations derived via statistical mechanics. This achieves a perfectly seamless connection between the atomistic and coarse-grained regions. In this talk we present simulations of the vibrational behavior of micron-scale oscillators. We find anomalous surface effects such as resonant frequency shifts and increased dissipation due to atomistic processes.

[1] J. Q. Broughton, et al., Phys. Rev. B 56, 611 (1997). [2] R. E. Rudd and J. Q. Broughton, "Atomistic Simulation of MEMS through the Coupling of Length Scales," in Proc. MSM '98 (Computational Publications, Boston, 1998) p. 287. [3] F. F. Abraham, et al., Comput. in Phys. 12, 538 (1998). [4] R. E. Rudd and J. Q. Broughton, Phys. Rev. B 58, R5893 (1998). [5] See URL: http://cst-www.nrl.navy.mil/~rudd/GrandChallenge
*with J. Q. Broughton

Mads Sorensen (LANL)*
Multiscale Materials Modeling in the Time Domain

The phrase ``multiscale materials modeling'' most often refers to multiple length scales and efforts to connect the atomistic and macroscopic scales. There is, however, a similar challenge in the time domain. Molecular dynamics (MD) simulations of the motion of the atoms in a material are usually limited to nanoseconds because of the short time step used in the numerical integration of the equations of motion. This is a problem because many important materials processes are activated processes that occur on a much longer time scale, i.e., microseconds or longer, beyond the reach of MD. In this talk we discuss a recently developed simulation method, temperature-accelerated dynamics, that can extend the time scale of dynamical simulations by taking advantage of the infrequent event nature of the processes. The method will be demonstrated for atomic diffusion on surfaces or at interfaces of metals.

*with Arthur F. Voter